Argonne-Northwestern Solar Energy Research (ANSER) Center
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The mission of the ANSER Center is to revolutionize our understanding of molecules, materials and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production. The ANSER Center will achieve this vision by understanding and characterizing the basic phenomena of solar energy conversion dynamics, by designing and synthesizing new nanoscale architectures with extraordinary functionality, and by linking basic solar energy conversion phenomena across time and space to create emergent energy conversion systems operating with exceptional performance. At the same time, the ANSER Center seeks to create and mentor a technically excellent workforce capable of solving energy-related problems far into the future. To achieve these goals, ANSER Center objectives are to develop a fundamental understanding of:

- the interaction of light and charge with molecules and materials
- the energy levels and electronic structures of molecules and materials
- the dynamics of photoinduced charge generation, separation, and transport with unparalleled temporal and spatial resolution
- the interfaces at which charge generation, separation, transport, and selective chemical reactions occur
- the properties of unique materials, from self-assembling, bio-inspired materials for hydrogen fuel production from water to transparent conductors and nanostructured hard and soft materials for solar electricity generation.

Subtask 1: Bio-inspired molecular materials for solar fuels. Natural photosynthesis is carried out by assemblies of photofunctional chromophores and catalysts within proteins, which provide specifically tailored nano-environments to optimize solar energy conversion. Achieving integrated artificial photosynthetic systems requires hierarchical organization at both molecular and supramolecular levels to capture light energy, separate charge, and transport charge to catalytic sites at which fuel synthesis occurs, e.g., H_2O oxidation to generate H_2. We do not yet understand in detail the basic scientific principles needed to build self-ordering, self-assembling components or the tailored nano-environments necessary to realize efficient, integrated artificial photosynthetic systems. The goals of Subtask 1 are to:

- Discover and utilize the fundamental scientific principles necessary to self-assemble biomimetic molecular systems to harvest light and perform photochemical charge separation.
- Discover and utilize the fundamental scientific principles necessary to couple photogenerated charges to multi-electron, multi-metallic catalysts for H_2O oxidation and H^+ reduction to H_2.
- Develop and utilize the fundamental understanding of how supramolecular assemblies and modified photosynthetic proteins can provide the tailored nano-environments necessary produce an integrated artificial photosynthetic system (e.g. Fig. 1).

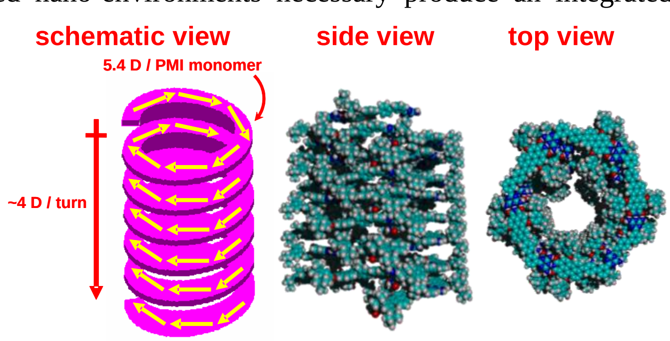

Fig. 1. Self-assembling nano-environment for integrated artificial photosynthesis.

Subtask 2: Interface science of organic photovoltaics. Organic photovoltaics (OPVs) offer the promise of low-cost, readily manufacturable alternatives to traditional inorganic systems for producing solar electricity. Power conversion efficiencies as high as 10-12% may be achievable, if crucial scientific understanding challenges can be surmounted. Progress requires a highly collaborative group, with experts in transparent conducting oxides (TCOs), in tailoring their interfaces with soft matter, in supramolecular assembly of charge-transporting arrays, and in applying an arsenal of state-of-the-art physical characterization and theoretical techniques. Subtask 2 combines unique, complementary expertise and resources, attacking key problems in OPV interface science in a comprehensive, integrated fashion, to achieve prototype cells which test enabling new concepts (e.g. Fig. 2). The resulting knowledge, materials, and techniques will be exploited in other types of interfaces necessary to implement the photodriven catalysts and solar cells in Subtasks 1 and 3, respectively.

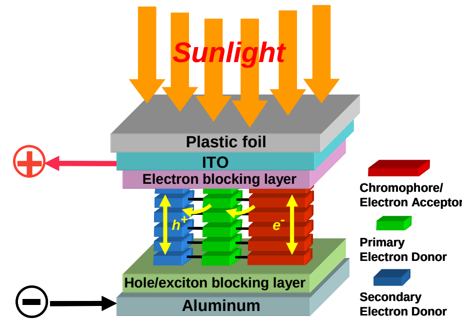

Fig. 2. A multilayer organic solar cell.

Subtask 3: Nanostructured architectures for photovoltaic and photochemical energy conversion. This subtask will define, develop, model, and test robust new nanostructured architectures, and associated new synthetic methodologies, that promise to advance substantially the science and technology of photovoltaic and photochemical solar energy conversion. Specifically, the subtask will focus on high surface area inorganic architectures capable of addressing key challenges in the design of exceptionally efficient Dye Sensitized Solar Cells (DSSCs) and highly functional fuel-producing solar cells (Subtask 1). This work will build on many of the activities in Subtasks 1 and 2 and synergistically provide information back to these subtasks. Dye-sensitized solar cells (DSSCs) represent one of the most promising alternatives to expensive silicon technology for conversion of solar radiation to electricity (Fig. 3a). Specifically, we will use new materials synthesis techniques to create conducting, semiconducting, and insulating oxide and metal nanostructures that can be used to systematically control key electronic, catalytic, and optical phenomena, and to favorably manipulate device dynamics and energetics. These structures will enable the plasmonic amplification of light harvesting ability, the use of energetically optimized redox shuttles that do not work in conventional architectures, and the coupling of photoelectrodes to fuel-forming catalysts (Fig. 3b).

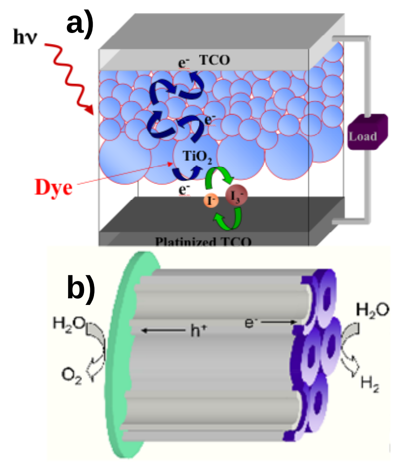

Fig. 3. a) DSSC based on electron injection into a wide bandgap, nanocrystalline, n-type semiconductor medium. **b)** *Compartmentalized* light-harvesting, catalytic oxidation, and catalytic reduction components function on a high-area, high-porosity, electrically conductive platform.

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